

1H-Benzimidazole, 2-phenyl-

Other names:	2-Phenylbenzimidazole Benzimidazole, 2-phenyl- Gainex Phenizidole Phenzidol Phenzidole 2-Phenyl-1H-benzimidazole G 570 2-Phenyl-1H-benzoimidazole NSC 251956
Inchi:	InChI=1S/C13H10N2/c1-2-6-10(7-3-1)13-14-11-8-4-5-9-12(11)15-13/h1-9H,(H,14,15)
InchiKey:	DWYHDSLWMUSOO-UHFFFAOYSA-N
Formula:	C13H9N2
SMILES:	c1ccc(-c2nc3ccccc3[nH]2)cc1
Mol. weight [g/mol]:	193.22
CAS:	716-79-0

Physical Properties

Property code	Value	Unit	Source
hsub	123.00 ± 1.70	kJ/mol	NIST Webbook
log10ws	-4.86		Crippen Method
logp	2.748		Crippen Method
mcvol	151.310	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.18	kJ/mol	572.20	NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C716790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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